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L5 STRUCTURE UPLOADED

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STRUCTURE FILE UPDATES: 22 SEP 2004 HIGHEST RN 749824-02-0 DICTIONARY FILE UPDATES: 22 SEP 2004 HIGHEST RN 749824-02-0

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=> s 15SAMPLE SEARCH INITIATED 19:37:25 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 174 TO ITERATE

100.0% PROCESSED

174 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

ONLINE \*\*COMPLETE\*\* FULL FILE PROJECTIONS: BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

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100.0% PROCESSED 3473 ITERATIONS SEARCH TIME: 00.00.01

1 ANSWERS

L7

1 SEA SSS FUL L5

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FILE COVERS 1907 - 23 Sep 2004 VOL 141 ISS 13 FILE LAST UPDATED: 22 Sep 2004 (20040922/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 4 L7

=> d fbib ab hitstr 1-4

- L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
- AN 2004:69052 CAPLUS
- DN 140:287333
- TI Facile synthesis of novel nonpeptide angiotensin II receptor antagonists
- AU Yang, Ling-Chun; Qi, Chuan-Min; Zhang, Guan-Xin; Zou, Nan-Zhi
- CS Department of Chemistry, Beijing Normal University, Beijing, 100875, Peop. Rep. China
- SO Journal of Heterocyclic Chemistry (2003), 40(6), 1107-1112 CODEN: JHTCAD; ISSN: 0022-152X
- PB HeteroCorporation
- DT Journal
- LA English
- OS CASREACT 140:287333
- 1-(Arylmethyl)-6-(methyloxazolyl)-4-methyl-2-propylbenzimidazoles such as AB I are prepared as analogs of the angiotensin II receptor antagonist Losartan. For example, I is prepared in ten steps from 3-methyl-4nitrobenzoic acid. Acid-mediated esterification of 3-methyl-4nitrobenzoic acid with methanol, Raney nickel-catalyzed reduction of the nitro group with hydrazine, acylation of the free amino group with butyryl chloride, nitration with fuming nitric acid, reduction of the nitro group with Raney nickel and hydrazine, and cyclocondensation yields the benzimidazolecarboxylate intermediate II. Hydrolysis of the Me ester of II, cyclocondensation with 4-methyl-3-aminophenol hydrochloride to yield the benzoxazole moiety, regioselective alkylation of the imidazole with Me 4-(bromomethyl)-1,1'-biphenyl-2'-carboxylate, and ester hydrolysis with sodium hydroxide in water yields I. The use of hydrazine as a reagent for the Raney nickel-catalyzed reduction of nitro groups is effective when the hydrazine is added in small amts. to avoid side reactions; the use of palladium or stoichiometric metal reductants could thus be avoided. The yield of the nitration of Me 4-(propylcarbonylamino)-3-methylbenzoate with fuming nitric acid is significantly improved with inverse addition of the amide to the nitric acid solution at -20°--15°. Alkylation of the benzoxazole-containing intermediate derived from II using sodium hydride as a base gives higher yields than in previous alkylations using sodium tert-butoxide as the base. The use of an ester-containing alkylating agent rather than a nitrile-containing alkylating agent allows milder conditions to be used for hydrolysis to the corresponding carboxylic acid, resulting in fewer byproducts.
- IT 301533-59-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1-(arylmethyl)-6-(methyloxazolyl)-4-methyl-2-propylbenzimidazole analogs of Losartan as potential nonpeptide angiotensin II receptor antagonists)

RN 301533-59-5 CAPLUS

CN Benzoic acid, 3-methyl-4-[(1-oxobutyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ C - OMe \\ \hline \\ n-Pr-C-NH & \\ Me \end{array}$$

## RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:889540 CAPLUS

DN 137:386311

TI Preparation and use of palladium catalysts for cross-coupling reactions

IN Rodefeld, Lars; Hopfner, Thomas; Reisinger, Claus-Peter

PA Germany

SO U.S. Pat. Appl. Publ., 8 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

PAN.	CNT I						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	US 2002173421	A1	20021121	US 2002-144080	20020513		
				DE 2001-10123884 A	20010516		
	DE 10123884	A1	20021121	DE 2001-10123884	20010516		
	EP 1260270	A1	20021127	EP 2002-9343	20020503		
	R: AT, BE, CH,	DE, DK	, ES, FR, G	B, GR, IT, LI, LU, NL, S	E, MC, PT,		
	IE, SI, LT,	LV, FI	, RO, MK, C	Y, AL, TR			
				DE 2001-10123884 A	20010516		
	JP 2003019436	A2	20030121	JP 2002-133832	20020509		
				DE 2001-10123884 A	20010516		
	CN 1385244	A	20021218	CN 2002-119915	20020516		
				DE 2001-10123884 A	20010516		

OS MARPAT 137:386311

AB Meterable solns. or dispersions of palladium catalysts Pd(Ar)L2X [Ar = (un)substituted aryl; L = phosphine ligand; X = anion] are manufactured by reacting (un)substituted chloroarom., bromoarom. or iodoarom. compds. or arenesulfonates with phosphine or diphosphine ligands and Pd salts. For example, refluxing a mixture of Pd(OAc)2 3.2, Ph3P 18.9 and 4-BrC6H4COMe for 1 h in 800 g 1,4-dioxane and stirring for 1 h at reflux temperature gave a title

catalyst solution Stirring p-BrC6H4CO2Me, CH2:CHCO2Me and NaOAc in Me2NAc in the presence of the above catalyst gave p-HO2CCH2C6H4CH:CHCO2Me in 72% yield.

IT 301533-59-5P

RL: IMF (Industrial manufacture); PREP (Preparation) (preparation and use of palladium catalysts for cross-coupling reactions)

RN 301533-59-5 CAPLUS

CN Benzoic acid, 3-methyl-4-[(1-oxobutyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ || \\ C - OMe \\ \\ N-Pr-C-NH \\ \\ Me \end{array}$$

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:730686 CAPLUS

DN 135:272759

TI Method for producing methyl 4-butanamido-3-methylbenzoate and the novel compound N-(4-bromo-2-methylphenyl) butanamide

IN Rodefeld, Lars; Hoepfner, Thomas; Klausener, Alexander; Behre, Horst

PA Bayer Aktiengesellschaft, Germany

SO PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

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λN . '	PAT	I FENT 1	NO.			KINI	)	DATE			APPI	LICAT	ION 1	. OI		D.	ATE		
[	WO 2001072690 WO 2001072690						,	WO 2001-EP2924				20010315							
		W:	AE, CO, HR, LT, RU,	AG, CR, HU, LU, SD,	AL, CU, ID, LV, SE,	AM, CZ, IL, MA, SG,	AT, DE, IN, MD, SI,	AU, DK, IS, MG, SK,	AZ, DM, JP, MK, SL,	DZ, KE, MN, TJ,	EE, KG, MW, TM,	BG, ES, KP, MX, TR,	FI, KR, MZ, TT,	GB, KZ, NO, TZ,	GD, LC, NZ, UA,	GE, LK, PL,	GH, LR, PT,	GM, LS, RO,	
		RW:	GH, DE,	GM, DK,	KE, ES,	LS, FI,	MW, FR,	MZ, GB,	SD, GR,	SL, IE, GW,	SZ, IT, ML,	TZ, LU, MR,	UG, MC, NE,	ZW, NL, SN,	AT, PT, TD,	SE, TG	TR,	BF,	
	DE	1001	5279			A1		2001	1004			-000					0000		
	UA	2001	0601	24		<b>A</b> 5		2001	1008		DE 2	2001- 2000- 2001-:	1001	5279	2	A 2		328	
		1268						2003	0102		EP 2	2001-	9337	03		2	0010	315	
	ΕP	1268						2004											
		R:						ES, RO,		CY,	AL, DE 2	TR 2000- 2001-	1001	5279	i	A 2	0000	328	
	JP	2003	5288	46		Т2		2003	0930		JP 2	2001-	5706	05		2	0010 0000	315	
	АТ	2732	70			E		2004	0815		AT 2	2001-: 2001 <b>-</b> 2000-	9337	03		2	0010 0010 0000	315	
	US	2003	0652	11		<b>A</b> 1		2003	0403		WO 2	2000- 2001-: 2002-:	EP29	24	1	w 2		315	

В2 20030916 US 6620962 A 20000328 DE 2000-10015279 W 20010315 WO 2001-EP2924 20030804 20040212 US 2003-633863 US 2004030183 Al A 20000328 DE 2000-10015279 W 20010315 WO 2001-EP2924 A3 20020924 US 2002-239678

OS CASREACT 135:272759; MARPAT 135:272759

AB The title ester (I, R = COOMe) is prepared in 3 steps from o-toluidine via I (R = Br).

IT 301533-59-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of Me 4-butanamido-3-methylbenzoate from toluidine)

RN 301533-59-5 CAPLUS

CN Benzoic acid, 3-methyl-4-[(1-oxobutyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel & \\ C-OMe \\ \hline \\ N-Pr-C-NH & \\ Me \end{array}$$

L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:738802 CAPLUS

DN 133:298017

TI Regioselective nitration of aniline derivatives and benzimidazoles therefrom

IN Schneider, Heinrich

PA Boehringer Ingelheim Pharma K.-G., Germany

SO Ger. Offen., 6 pp. CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

twi.	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
PI	DE 19917524	A1 20001019		19990417
	DE 19917524 WO 2000063158	C2 20010920 A1 20001026		20000412
	W: CA, JP, M	K, US		
	RW: AT, BE, CH PT, SE	H, CY, DE, DK, ES,	FI, FR, GB, GR, IE, I	T, LU, MC, NL,
	11, 55		DE 1999-19917524	A 19990417
	EP 1173407	A1 20020123	EP 2000-917076	20000412
		H, DE, DK, ES, FR,	GB, GR, IT, LI, LU, N	L, SE, MC, PT,
	IE, FI		DE 1999-19917524	A 19990417
			WO 2000-EP3247	W 20000412
	JP 2002542222	T2 20021210	JP 2000-612254	20000412
			DE 1999-19917524	A 19990417
			WO 2000-EP3247	W 20000412

OS MARPAT 133:298017

- The highly regioselective nitration of 4-(alkanoylamino)-3-alkylbenzoic acid esters in the 5-position is carried out using a mixture of sulfuric and nitric acids followed by a subsequent addition of nitric acid alone. The nitro group may be reduced to an amine group and the product then converted to a benzimidazole. Thus, Me 4-(butyrylamino)-3-methylbenzoate was nitrated with a mixture of sulfuric and nitric acids, with further addition of nitric acid to give 91% Me 4-(butyrylamino)-3-methyl-5-nitrobenzoate virtually free os isomers. Procedures employing no second addition of nitric acid or using sulfuric acid alone followed by a nitric-sulfuric acid mixture resulted in an appreciable amount of the 2- and 6-nitro isomers.
- RN 301533-59-5 CAPLUS
  CN Benzoic acid, 3-methyl-4-[(1-oxobutyl)amino]-, methyl ester (9CI) (CA
  INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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